AGH UNIVERSITY OF SCIENCE AND TECHNOLOGY

Module name: Computational materials science

Academic year: 2019/2020 Code: ZSDA-3-0002-s ECTS credits: 3

Faculty of: Szkoła Doktorska AGH

Field of study: Szkoła Doktorska AGH Specialty: —

Study level: Third-cycle studies Form and type of study: Full-time studies

Lecture language: English Profile of education: Academic (A) Semester: 0

Course homepage: http://home.agh.edu.pl/~lmadej/

Responsible teacher: Madej Łukasz (lmadej@agh.edu.pl)

Module summary

This lecture is devoted to introduction into the computational materials science. The first part of the lecture is devoted to presentation of macro, micro, mezo and nano scale numerical modeling techniques. Practical basis of the commonly used methods are presented. Their advantages as well as disadvantages are discussed. The second part of the lecture is focused on examples of capabilities offered by advanced modelling techniques in the area of material and process development.

Description of learning outcomes for module

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Connections with FLO	Method of learning outcomes verification (form of completion)
Social competence: is able to			
M_K001	Can appreciate the advantages of the use of modeling techniques to develop new materials and technologies that can be useful for the society.	SDA3A_K02	Presentation, Oral answer
Skills: he can			
M_U001	Has the ability to identify parameters of the material model.	SDA3A_U01	Oral answer
Knowledge: he knows and understands			
M_W001	Has general knowledge about the advantages and possibilities of application of numerical modeling techniques in material science and engineering.	SDA3A_W03, SDA3A_W02	Presentation, Oral answer

M_W002	Has general knowledge on selection of appropriate methods of macro, meso, micro and nano scale analysis to solve problem under consideration.	SDA3A_W03, SDA3A_W02	Presentation, Oral answer

Number of hours for each form of classes

	Form of classes										
Suma	Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
20	12	0	0	0	0	8	0	0	0	0	0

FLO matrix in relation to forms of classes

MLO code	Student after module completion has the knowledge/ knows how to/is able to	Form of classes										
		Lectures	Auditorium classes	Laboratory classes	Project classes	Conversation seminar	Seminar classes	Practical classes	Fieldwork classes	Workshops	Prace kontrolne i przejściowe	Lektorat
Social competence: is able to												
M_K001	Can appreciate the advantages of the use of modeling techniques to develop new materials and technologies that can be useful for the society.	+	-	-	-	-	-	-	-	-	-	-
Skills: he can												
M_U001	Has the ability to identify parameters of the material model.	+	-	-	-	-	+	-	-	-	-	-
Knowledge: he knows and understands												
M_W001	Has general knowledge about the advantages and possibilities of application of numerical modeling techniques in material science and engineering.	+	-	-	-	-	-	-	-	-	-	-
M_W002	Has general knowledge on selection of appropriate methods of macro, meso, micro and nano scale analysis to solve problem under consideration.	+	-	-	-	-	+	-	-	-	-	-

Student workload (ECTS credits balance)

Student activity form	Student workload
Udział w zajęciach dydaktycznych/praktyka	20 h
Preparation for classes	20 h
przygotowanie projektu, prezentacji, pracy pisemnej, sprawozdania	20 h
Realization of independently performed tasks	15 h
Contact hours	2 h
Summary student workload	77 h
Module ECTS credits	3 ECTS

Additional information

Module content

Lectures

Computational material science – introduction

Macro scale analysis techniques

Mezo scale analysis techniques

Micro and nano scale analysis techniques

Multi scale analysis techniques

Scientific and industrial applications of the multi scale approaches

Seminar classes

Capabilities of numerical modelling techniques – case studies 1

Capabilities of numerical modelling techniques – case studies 2

Capabilities of numerical modelling techniques – case studies 3

Capabilities of numerical modelling techniques – case studies 4

Teaching methods and techniques:

Lectures: Oral presentation, multimedia presentation, animations
Seminar classes: Oral presentation, multimedia presentation,

Warunki i sposób zaliczenia poszczególnych form zajęć, w tym zasady zaliczeń poprawkowych, a także warunki dopuszczenia do egzaminu:

-Participation in the classes
-Positive grade from the project

Zasady udziału w poszczególnych zajęciach, ze wskazaniem, czy obecność studenta na zajęciach jest obowiązkowa:

Lectures:
– Attendance is mandatory: No
– Participation rules in classes: Participation in the classes is mandatory
Seminar classes:
– Attendance is mandatory: Yes
– Participation rules in classes: Participation in the classes is mandatory

Method of calculating the final grade
Grade from classes will be the basis of the final mark.

Sposób i tryb wyrównywania zaległości powstałych wskutek nieobecności studenta na zajęciach:
Will be discussed during the first class.

Prerequisites and additional requirements
Basic knowledge of materials science.

Recommended literature and teaching resources
1. Pietrzyk M., Madej L., Rauch L., Szeliga D., Computational Materials Engineering: achieving high accuracy and efficiency in metals processing simulations, Butterworth-Heinemann Elsevier, 2015.
2. O. C. Zienkiewicz, R. L. Taylor, The Finite Element Method Set, Butterworth-heinemann, 2005.
3. Fries T.P., Matthies H.G., Classification and overview of meshfree methods, Scientific Computing, Informatikbericht, 2003-3, Brunswick, 2004.

Scientific publications of module course instructors related to the topic of the module
1. Madej L., Mojżeszo M., Chraponski J., Roskosz S., Cwajna J., Digital material representation model of porous microstructure based on 3D reconstruction algorithm, Archives of Metallurgy and Materials, 62, 2017, 563-569.
2. Madej L., Digital/virtual microstructures in application to metals engineering – A review, Archives of Civil and Mechanical Engineering, 17, 2017, 839–854.
3. Madej L., Legwand A., Mojzeszko M., Chraponski J., Roskosz S., Cwajna J., Experimental and numerical two- and three-dimensional investigation of porosity morphology of the sintered metallic material, Archives of Civil and Mechanical Engineering, 18, 2018, 1520-1534.
4. Madej L., Mabrozinski M., Kwiecień M., Gronostajski Z., Pietrzyk M., Digital material representation concept applied to investigation of local inhomogeneities during manufacturing of magnesium components for automotive applications, International Journal of Materials Research, 108, 2017, 3-11.
5. Szyndler J., Grosman F., Tkocz M., Madej L., Numerical and experimental investigation of the innovatory incremental forming process dedicated for the elaerospace industry, Metallurgical and Material Transactions A, 11, 2016, 5522-5533.

Additional information
None